

A Theory of DDT in Unconfined Flames

Alexei M. Khokhlov,* Elaine S. Oran,** J. Craig Wheeler*

* Department of Astronomy
University of Texas at Austin
Austin, TX 78712

** Laboratory for Computational Physics
Naval Research Laboratory
Washington, DC 20375

Corresponding Author:

Dr. Alexei M. Khokhlov
Department of Astronomy
University of Texas at Austin
Austin, TX 78712
phone: 512-471-3397
fax: 512-471-6016
e-mail: ajk@astro.as.utexas.edu

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Alexei M. Khokhlov,* Elaine S. Oran,** J. Craig Wheeler*

* Department of Astronomy
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Abstract

This paper outlines a theoretical approach for predicting the onset of detonation in unconfined turbulent flames. Two basic assumptions are made: 1) the gradient mechanism is the inherent mechanism that leads to DDT in unconfined conditions, and 2) the sole mechanism for preparing the gradient in induction time is by turbulent mixing and local flame quenching. The criterion for DDT is derived in terms of the one-dimensional detonation wave thickness, the laminar flame speed, and the laminar flame thickness in the reactive gas. This approach gives a lower-bound criterion for DDT for conditions where shock preheating, wall effects, and interactions with obstacles are absent. Regions in parameter space where unconfined DDT can and cannot occur are determined.

1. Introduction

The quantitative prediction of deflagration-to-detonation transition (DDT) in energetic gases is one of the major unsolved problems in combustion and detonation theory. Predicting the occurrence of DDT has practical importance because of its destructive potential. It is also an extremely interesting and difficult scientific problem because of the complex nonlinear interactions among the different contributing physical processes, such as turbulence, shock interactions, and energy release. An early description of experiments on DDT is given by Brinkley and Lewis [1], who also describe Karlovitz's theory [2]. Much of this theory has subsequently been experimentally confirmed and expanded upon by Oppenheim and coworkers [3–5]. Excellent reviews that summarize our understanding to date have been given by Lee and Moen [6] and, most recently, by Sheppard and Lee [7]. Other useful summaries of mechanisms of DDT have been given by Lewis and von Elbe [8] and Kuo [9].

Turbulence plays an important role in DDT. Several apparently different mechanisms for the DDT in confined conditions have been described, each including the turbulence of the flame and formation of shocks. On large scales, turbulence deforms the flame front and increases its surface area. On small scales, it broadens the flame front and causes mixing. The result is an extended turbulent “flame brush” in which a series of explosions occurs, one of which finally leads to a detonation. Other routes to detonation may include an explosion in the boundary layer, or an explosion inside the region between the leading shock and flame brush.

It is believed that, in most cases, the intrinsic mechanism triggering a detonation is the explosion of a nonuniformly preconditioned region of fuel in which a spatial gradient of induction time has been created either by turbulent mixing, shock heating, or both. This gradient mechanism, first suggested by Zeldovich and collaborators for nonuniform temperature distributions [10,11], was subsequently found in photo-initiation experiments by Lee et al. [12], who called it the SWACER mechanism. This mechanism has since been studied and described extensively (see, for example, [6,13–16]). The mechanisms for preconditioning the region, that is, the mechanism for preparing an explosive mixture that has a gradient in induction times, may differ in different situations. It may be created by a shock wave, turbulence, photo-irradiation, intrinsic flame instabilities, rarefaction, or a combination of several of these.

It appears to be very difficult to obtain DDT in unconfined conditions [17–19]. This can be attributed to the geometrical effects of expansion: shocks which precede a deflagration might be weakened, or turbulence might be damped too much by the expansion, and so become unable to precondition the mixture. Wagner and coworkers [17] report experiments in which deflagrations were forced to DDT by passing through screens of specified mesh sizes. The screens created turbulence of the required scale and intensity. These experiments suggest that an unconfined deflagration could make the transition to detonation under the right conditions. This possibility has been suggested for very large vapor clouds [6,20].

A related problem that has been studied experimentally is initiation of detonations by turbulent jets [18,21–24]. In these experiments, a jet of hot product gases is injected into an unburned, cold mixture. The turbulence generated by the interaction of this jet and the background gas created a nonuniform, preconditioned region in which detonation may occur. For these experiments, the effects of reflected shocks and interaction with walls is minimal compared to DDT in tubes. Therefore, these experiments provide important information on the critical size of the region capable of triggering DDT.

We then ask the following question: What are the minimal requirements for DDT in an

idealized situation when all wall effects and incident shocks are eliminated? If we can answer this question, we have a lower bound for DDT conditions. Knowing the necessary conditions for unconfined DDT, we may then draw conclusions about the relative importance of wall effects and shocks of different strengths. One possible application of this theory could be to create reproducible detonations in the shortest time and smallest space, as required for pulse-detonation engines. Another application is to the theory of supernovae. If DDT does occur in supernovae, as indicated by observations [25,26], it would arise from an unconfined transition. Currently, there is no quantitative theory explaining exactly how and when an unconfined transition would occur.

In this paper, we derive a theory for unconfined DDT. That is, we address the situation where there are no external or reflected shocks, and no wall effects. We make two basic assumptions:

- i.* The gradient mechanism is the inherent mechanism that leads to DDT in unconfined conditions, and
- ii.* The sole mechanism for preparing the gradient in induction time is by turbulent mixing and local flame quenching. By this assumption, the role of turbulence is to mix high-entropy products of burning and low-entropy unreacted fuel. Such mixing creates gradients of temperature and concentration which have opposite signs. Turbulence-generated shocks are ignored.

Given these assumptions, there are two fundamental questions to address: 1) What is the minimum size of a mixed region capable of generating a detonation, and 2) What level of turbulence is required to create this region? We address these two questions separately, and then combine the answers to derive the conditions for unconfined DDT. Here we do not address the question how these conditions may be produced, but give the scale and intensity of the turbulence that is required. The derived criterion gives *lower bounds* on conditions for DDT that does not take into account many secondary effects that may facilitate DDT. We then conclude with a discussion of the quantitative importance of secondary effects.

2. Critical Size of the Preconditioned Region

In this section we address the first of the two questions formulated in the introduction. We consider the process of the initiation of detonation that arises from the explosion of reactive gas with a nonuniform distribution of induction times. We assume that the nonuniformity is a result of mixing of high-entropy products and low-entropy unreacted fuel. We determine the minimum size L_c of a mixed region capable of triggering a detonation. Whether and how such a region can be created is a separate question that is studied in Section 3.

We can imagine a variety of regions of different shapes and degrees of mixing created by turbulence. Here we consider the simplest representative case of a mixed region with a *linear* one-dimensional distribution of products. In the future, we plan to consider regions with different shapes, and thus explore the influence of geometry. However, we do not believe geometrical considerations will qualitatively change our conclusions (Section 3.2).

2.1 Spontaneous Burning

To facilitate the discussion of a nonuniform explosion of a mixed region, it is useful to discuss in general terms the idea of spontaneous burning. This concept was first introduced in Zeldovich and Kompaneetz [27]. Consider a mixture with a nonuniform distribution of temperature $T(x)$ and chemical composition $Y(x)$. The induction time becomes a function of spatial coordinate, $\tau(T(x), Y(x))$. In the absence of any physical communication between different fluid elements, the explosion will start at a point of minimum τ , and then will spread spontaneously with a “phase” speed

$$D_{sp} = \left(\frac{d\tau}{dx} \right)^{-1}, \quad (1)$$

which can have any value from zero to infinity. A spontaneous reaction wave does not require any physical agent in order to spread. Therefore, its speed is not limited by the speed of light. In reality, there is physical communication between fuel elements. If the spontaneous velocity is too small, shocks and even heat conduction may cause faster flame propagation than that prescribed by equation (1).

Let δt be the time during which the bulk of chemical energy is released after the induction period is over, $\delta t \ll \tau$. We can define the thickness of the spontaneous wave as $l_{sp} \simeq D_{sp} \delta t$. If $D_{sp} \rightarrow \infty$, the thickness of the wave also goes to ∞ . This corresponds to a constant volume explosion. If D_{sp} is comparable to the speed of a detonation, on the other hand, its thickness is also comparable to the thickness of a detonation wave. In this latter case, δ_{sp} may become much less than the size of the system under consideration. Then the

spontaneous wave may be viewed as discontinuity which obeys the Hugoniot relations for a discontinuity with energy release.

On a pressure – specific volume plane, spontaneous burning is represented by points located on a detonation adiabat. This is shown on Figure 1a, where the regimes of spontaneous burning occupy the part of the detonation adiabat from point I to point CJ. The position of the spontaneous regime on the adiabat is determined by the intersection of the Rayleigh line $dP/dV = -(D_{sp}/V_0)^2$ with the detonation adiabat. The regime I corresponds to an infinite spontaneous velocity when all matter burns simultaneously due to uniform preconditioning. The point CJ corresponds to the minimum possible velocity of a steady spontaneous wave, and is equal to the Chapman-Jouguet velocity of a steady detonation. The same part of the detonation adiabat, I – CJ, is occupied by weak detonations. The difference between spontaneous waves and detonations, is that there is no shock wave present inside a spontaneous wave. The structure of a Chapman-Jouguet detonation and a spontaneous wave of the same strength is shown schematically in Figure 1b.

In a detonation, the material is first shocked (point S in Figure 1), and then expands towards the CJ point along the S – CJ line. In the corresponding spontaneous wave, the material is continuously compressed along the O – SP line until it reaches the CJ point (or some other point SP). The pressure, density, and velocity in a spontaneous wave become larger than those of a constant volume explosion (point I) because burning does not proceed simultaneously! There exists a pressure gradient inside the wave pointing opposite to its direction of propagation, since at any instant the wave consists of fluid elements with different amounts of released energy. As a result, a fluid element passing through the wave is compressed and accelerated by this gradient. The slower the wave moves, the longer is the time spent inside the wave, and the greater are the pressure, density and velocity jumps across the wave. The principle of causality is not violated in the spontaneous wave, as explained in [28]. Although the speed of the spontaneous wave is a phase speed, it is a real supersonic wave of burning which looks like a detonation in terms of the hydrodynamic parameters of burned material.

We have discussed the situation where the spontaneous wave speed is greater or equal to the CJ detonation velocity, D_{CJ} . Suppose the gradient in induction time is such that D_{sp} is initially greater than D_{CJ} , but then it decreases so that it becomes less than D_{CJ} . In this case, when the spontaneous wave crosses the CJ threshold, the burned material immediately behind the wave, which moves with the local sound speed relative to the wave, will tend to overcome the wave and produce a shock. Consider an intermediate regime with such a shock, O – O' – S' – CJ, shown in Figure 1. First, material burns in a spontaneous

wave from O – O', then it is shocked to point S', and then returns to the CJ point. The transition from the spontaneous wave to a CJ detonation may then proceed through a sequence of such regimes, with increasing shock strengths.

The description given in the last paragraph is a quasi-steady picture that is applicable only if the spontaneous wave velocity changes slowly enough. If the spontaneous wave velocity changes too fast, that is, the gradient is too steep, the shock and reaction will separate, and the CJ detonation will not form. In the process of transition from spontaneous wave to CJ detonation, the spontaneous velocity must change slowly enough so that the shock and reaction do not separate. This means that the nonuniform region must be large enough so that this separation does not occur, and this, in turn, gives a criterion for unconfined DDT.

2.2 Formulation of the Problem

Consider an idealized one-dimensional system with the equation of state $P = (\gamma - 1)E_t$ and $T = P/\rho$, where P , T , ρ and E_t are the pressure, temperature, mass density and thermal energy density, respectively. The chemical reaction is described by a first-order Arrhenius expression,

$$\frac{dY}{dt} = -Y \exp\left(-\frac{Q}{T}\right), \quad (2)$$

where Q is the activation energy, and the chemical variable Y ranges from $Y = 1$ for pure reactants to $Y = 0$ for total products. Units of distance and time are such that the pre-exponential factor in equation (1) is unity, and the gas constant is $R = 1$. Planar geometry is assumed. The system obeys the Euler equations,

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho U) &= 0, \\ \frac{\partial \rho U}{\partial t} + \frac{\partial}{\partial x}(\rho U^2 + P) &= 0, \\ \frac{\partial E}{\partial t} + \frac{\partial}{\partial x}((E + P)U) &= 0, \end{aligned} \quad (3)$$

where U is the fluid velocity, $E = E_t + \rho U^2/2 - \rho qY$ is the total energy density including chemical energy, and q is the total energy release per unit mass.

The initial temperature and density of the fuel are T_0 and ρ_0 . The products of isobaric burning, an approximation to burning in a laminar flame, have a temperature $T_1 = T_0 + q\left(\frac{\gamma-1}{\gamma}\right)$. By our assumption, we consider a nonuniform region created by *mixing* the products of isobaric burning and fresh fuel, such that there is a linear spatial distribution

of reactants $Y(x)$ and temperature $T(x)$,

$$\begin{aligned} Y(x) &= \begin{cases} x/L, & 0 \leq x \leq L \\ 1, & x > L \end{cases} \\ T(x) &= T_1 - (T_1 - T_0) Y(x) , \end{aligned} \quad (4)$$

where L is the size of the mixed region. Initially, the velocity of the material is zero, and the pressure P_0 is constant everywhere. The boundary conditions at $x = 0$ are reflecting walls (symmetry conditions).

The system is prepared in an initial state and then evolves in time, first until ignition takes place, then to the formation (or failure) of detonation, and then to the time when the generated detonation or shock leaves the computational domain. The cases considered are listed in Table 1. Parameters for the standard case H1 with $P_0 = 1$ and $T_0 = 1$ are chosen to approximate a detonation in a stoichiometric hydrogen and oxygen mixture at pressure of 1 atm and temperature of 293 K [29,30]. The extra cases, H2 ($T_0 = 2$) and H3 ($T_0 = 3$), are considered to study the sensitivity of the detonation formation to the initial temperature of the fuel.

The system of equations (2) and (3) is integrated numerically using a one-dimensional version of a time-dependent, compressible fluid code based on the Piecewise Parabolic Method (PPM) [31,32]. PPM is a second order Godunov-like method which incorporates a Riemann solver to describe shock waves accurately. Shocks are typically spread on one or two computational cells wide. A piecewise parabolic advection algorithm advects sharp shockless features, such as density and composition discontinuities or gradients, without diffusing them excessively or changing their shape. Contact discontinuities are typically kept two or three cells wide. Details of the implementation are given in [33,34]. The chemical reaction is coupled to fluid dynamics by time-step splitting. The kinetic equation (2) is integrated together with the equation of energy conservation using adjustable substeps to keep the accuracy better than 1%. The grid spacing is selected so that there are at least 10 cells within a detonation wave reaction zone. The convergence of numerical solutions was thoroughly tested by varying the number of computational cells from 1024 to as many as 65536 in some cases.

2.3 Detonation Formation Inside the Mixed Region

The induction time τ as a function of temperature T and fuel fraction Y can be expressed as

$$\tau(T, Y) \simeq \frac{1}{(\gamma - 1)qY} \left(\frac{T^2}{Q} \right) \exp \left(\frac{Q}{T} \right) \quad (5)$$

using the Frank-Kamenetskii approximation [35], valid when $T/Q \ll 1$, and assuming the induction takes place at constant volume. The derivatives of τ with respect to T and Y are

$$\frac{\partial \tau}{\partial T} \simeq -\frac{\tau Q}{T^2}, \quad \frac{\partial \tau}{\partial Y} \simeq -\frac{\tau}{Y}. \quad (6)$$

For the mixture considered here, the values of T and Y are related by equation (4). The function $\tau(T, Y(T))$ then has a minimum at T_m , found by solving $d\tau/dT = \partial\tau/\partial T + (\partial\tau/\partial Y)(dY/dT) = 0$, so that

$$T_m^2 + QT_m - QT_1 = 0. \quad (7)$$

This gives

$$\begin{aligned} T_m &= Q \frac{\sqrt{1 + 4\frac{T_1}{Q}} - 1}{2} \simeq T_1 \left(1 - \frac{T_1}{2Q}\right), \\ x_m &= L \left(\frac{T_1 - T_m}{T_1 - T_0}\right) \simeq \frac{LT_1}{2Q}, \end{aligned} \quad (8)$$

for $T_0 \ll T_1$. The point x_m is the first to ignite. From this point, a spontaneous reaction wave propagates with the speed

$$D_{sp} = \left(\frac{d\tau}{dx}\right)^{-1} = \frac{T^2(T - T_1)}{(T_1 - T_0)(T^2 + QT - QT_1)} \frac{L}{\tau}. \quad (9)$$

By virtue of equation (7), the speed of the reaction wave is infinite at point x_m . Thus, the reaction wave initially propagates supersonically, as described in Section 2.1. We are interested in the propagation of the wave to the right, $x \rightarrow L$, where the energy released by the wave increases. The velocity of the wave decreases towards larger x , and becomes equal to the local sound speed at some point x_s determined by

$$D_{sp}(x_s) = D_{CJ}. \quad (10)$$

At this point, a pressure wave forms which runs into the mixture ahead of the decelerating reaction wave. Whether this pressure wave is strong enough to accelerate burning and to evolve into a detonation wave depends on the length L of the mixed region.

There are two processes involved in the transformation of the pressure wave into a detonation. First, the pressure wave must steepen into a shock. This shock must accelerate burning so that a shock–reaction complex forms. Second, the shock–reaction complex must survive the propagation down the temperature gradient. We denote as L_s the first critical length of the mixed region such that for $L < L_s$ the shock–reaction complex does not form.

For $L > L_s$, the shock–reaction complex successfully forms within the mixed region. We denote as L_d the second critical length of the mixed region such that for $L > L_d$, the shock–reaction complex survives and passes as a detonation into the cold fuel. For $L_s < L < L_d$, the shock–reaction complex dies inside the mixed region.

Values of L_s and L_d were determined by the numerical simulations described in Section 2.2 by performing a series of simulations in which the size L of the mixed region was varied. Figures 2–5 show results of simulations for H1 for four different choices of L . Each figure shows the evolution with time of the pressure, velocity, temperature, and reactant concentration. Figure 2 shows the results for the smallest mixed region, $L = 30x_d$, where x_d is the half-reaction width of a CJ detonation. This region is so small that the quasi-steady spontaneous wave cannot form. The pressure wave is too weak to form a shock–reaction complex. The pressure wave generated by the spontaneous burning steepens into a shock outside of the mixed region.

For $L = 300x_d$, shown in Figure 3, a shock wave forms at the point predicted by equation (10), and the complex forms. The simulations show that the shock–reaction complex is far from a steady CJ detonation and cannot be described as a small quasi-steady deviation from the CJ state. The peak pressure is at least a factor of two less than the von Neumann pressure for the equivalent CJ detonation at the local condition. Figure 3 shows that, soon after the complex is formed, the reaction zone and shock wave separate, and only a shock wave leaves the mixed region. This is because the shock–reaction complex, after being formed, must propagate through the mixture with continuously decreasing temperature. The temperature gradient causes rapid decrease in the postshock temperature, and, consequently, rapid growth of the induction time in the postshock material.

Figures 4, $L = 500x_d < L_d$, shows a case similar to Figure 3, but the shock–reaction complex decouples close to the end of the mixed region. In Figure 5, $L = 960x_d > L_d$, the complex transforms into a detonation, and passes into the cold unmixed fuel. The critical condition for the initiation of detonation in mixed fuel and products is that the shock–reaction zone complex survives its propagation through the temperature gradient. The critical lengths, L_d , of a region capable of triggering a detonation, as determined by such simulations, are presented in Table 1 for cases H1 – H3.

The value of the critical length L_d is sensitive to initial temperature T_0 . An increase of T_0 facilitates the initiation of detonation. Cases H2 and H3 in Table 1 show that L_d decreases by a factor of six if the initial temperature is tripled. This can be explained if the criterion for the detonation formation is not the creation, but rather the survival of the shock–reaction complex. For higher initial temperature, the postshock induction time is

less sensitive to variations of background conditions (see equation 6), and so it is easier for the shock–reaction complex to adjust to changing conditions.

2.4 Relation to Jet Initiation Experiments

One possible check on the theory described above for determining L_d is to compare the predictions of Section 2.3 with the results of turbulent jet-initiation experiments [18,21–24]. In these experiments, a jet of hot product gases is injected into an unburned, cold mixture. The jet can be characterized by the size of the orifice, d , through which hot products are injected. The turbulence caused by the interaction of this jet and the background gas creates a nonuniform, preconditioned region in which detonation may occur. The largest scale of the turbulence and the size of the mixed region are also characterized by d . For these experiments, the effects of reflected shocks and interaction with walls is believed to be small. The velocity of the jet is approximately sonic with respect to the unburned background material. Thus the strengths of the shocks formed by the exiting jet resulted in overpressures in the unburned gas of about a factor of two or less. The temperature increase was small. Ignition occurred in the jet and seemed to be unaffected by wall interactions.

Depending on d , two distinct ignition regimes were found. For small d , deflagrations were ignited at many points inside the mixed region. There was no transition to detonation. For larger d , there was an explosion in the mixed region that led to detonation. From these experiments, the minimum value of d for which DDT occurred was $d > 10 - 20l_c$, where l_c is the detonation cell size.

The half-reaction zone length x_d , in terms of which we derived our estimates of L_d , is a theoretical parameter. What is measured in experiments is a detonation cell size l_c . In order to estimate l_c for the case H1, we use the results of two-dimensional simulations of detonation cell structure for conditions similar to H1 [30]. Scaling the results of these simulations to nondimensional units, we find $l_c \simeq 27x_d$, where we have taken l_c to be the height of a detonation cell. That is, the critical size of the mixed region in case H1 is $L_d \simeq 36l_c$. Thus the theoretical estimate of L_d is in qualitative agreement with experiments. The somewhat larger theoretical value, $36l_c$ compared to $10 - 20l_c$, could be the result of the simplifying assumptions (one-step kinetics, neglect of multi-dimensional effects) made in this paper.

There have been other efforts to relate L_d to l_c . For example, Knystautus et al. [18] found that $L_d \simeq 13l_c$ based on the analogy between DDT and direction initiation of detonation by an energy source. Dorofeev et al. [21] report $L_d > 7l_c$ based on their computations.

3. Critical Turbulent Velocity for DDT

3.1 Preconditioning by Turbulence

The discussion in the previous section established that the size of the region required to trigger a detonation is large compared to the one-dimensional detonation thickness, $L_d \simeq 10^3 x_d$ for case H1. Now the question is how to create this region. In an unconfined space, turbulence is the only mechanism available. The turbulence in the region of size L_d must be strong enough to create microscopic mixing in this region. Turbulence on large scales must be intense enough to pack individual laminar flame sheets close together. Turbulence on small scales must be strong enough to broaden and destroy individual flame sheets so that the products and fuel can mix to form a microscopic region with a gradient of induction times.

There are generally two regimes of turbulent flames we need to consider. The first is a regime of multiple flame sheets, in which the flame is irregular on large scales but laminar on small scales. The second is the distributed burning regime, in which the turbulence is so strong that it modifies the laminar flame structure (See, for example [36,37]. The transition between the multiple flame sheet and distributed burning regimes represents the condition where the creation of the large-scale nonuniform distribution of induction times becomes possible. The flame will be affected by the turbulence on scales $\lambda \geq \lambda_G$, on which the turbulent velocity is greater than or equal to the laminar flame speed, S_l . Here λ_G is the Gibson scale defined by the condition

$$U(\lambda_G) = S_l \quad (11)$$

where $U(\lambda)$ is the turbulent velocity on the scale λ . The transition between the two turbulent regimes happens approximately when λ_G approaches the thickness of the laminar flame x_l [36]. This estimate is approximate and does not account for the effects of viscosity, which becomes important when λ_G approaches the viscous microscale λ_K . The viscosity destroys turbulent eddies of size x_l . Poinot et al. [38] have shown theoretically that because of this effect, eddies larger than λ_G with velocity greater than S_l are needed to quench the flame. This has been substantiated by the experimental work by Roberts and Driscoll [39] who showed that eddies a factor of four larger are required.

Consider, for simplicity, a Kolmogorov cascade inside the turbulent flame brush such that on the scale λ , the turbulent velocity is

$$U_\lambda \simeq U_\mathcal{L} \left(\frac{\lambda}{\mathcal{L}} \right)^{1/3}, \quad (12)$$

where \mathcal{L} is the driving scale of the turbulence, which could be approximately equal to or larger than the size of the turbulent flame brush, and $U_{\mathcal{L}}$ is the turbulent velocity on this scale. In this case, the Gibson scale λ_G becomes

$$\lambda_G \simeq \left(\frac{S_l}{U_{\mathcal{L}}} \right)^3 \mathcal{L}. \quad (13)$$

The condition $\lambda_G = x_l$ now can be used to define the intensity of the turbulent motions needed for DDT,

$$U_{\mathcal{L}} = K S_l \left(\frac{\mathcal{L}}{x_l} \right)^{1/3}, \quad (14)$$

where we introduced a coefficient $K \simeq 1$ which describes the ability of the laminar flame to survive stretching and folding caused by turbulence on scales of the order of x_l . Once the condition of equation (14) is reached for $\mathcal{L} \geq L_d$, DDT can occur by the gradient mechanism.

For a typical flame, the thickness of the laminar flame x_l is approximately an order of magnitude less than x_d . That is, $L_d \simeq 10^4 x_l$. For a flame with $L_d/x_l = 10^4$, the intensity of turbulent motions required for DDT on the scale of L_d must be about $U_{L_d} \simeq 20 S_l$, as follows from equation (14). For example, consider an equimolar acetylene-oxygen flame with a laminar flame speed of 5 m/s [40]. From equation (12), the critical intensity of turbulent motions is approximately $U_{\mathcal{L}} \simeq 100$ m/s. The critical turbulent velocity could be considerably less in confined conditions because of the presence of shocks.

In unconfined situations, there are two possible sources of turbulence, the Landau-Darrieus (L-D) instability and the Rayleigh-Taylor (R-T) instability. The L-D instability is an intrinsic hydrodynamic flame instability that does not require external acceleration. The intensity of the L-D induced turbulent motions is unlikely to be much larger than S_l because of nonlinear stabilization effects [41]. The L-D instability is thus not likely to produce the level of turbulence required for DDT in any reasonable conditions. The characteristic turbulent velocity associated with the R-T instability on scale L is of the order of $\simeq \sqrt{gL} \simeq 3\sqrt{L}$ m/s for L in meters. The level of turbulence required for DDT can thus be achieved only on scales of ~ 100 m. This could explain why DDT in unconfined situations is so rarely observed. To obtain DDT in the laboratory, we need some other way of inducing much higher turbulent intensities.

3.2 Secondary Effects

When a region smaller than L_d ignites, it can still generate a substantial shock. The dependence of the maximum shock pressure on L found from the simulations is shown in

Figure 6. The shock strength is high for L larger than, say, $0.5L_d$, but rapidly decreases for smaller L . There are two possible effects these shocks may produce, one related to the temperature increase and another to vorticity created by the shocks.

The shock may raise the temperature in a region of the mixture that is about to explode, and this may facilitate the survival of the shock–reaction complex. Table 1 shows that the increase of the initial temperature from $T_0 = 1$ to $T_0 = 2$ decreases L_d by a factor of four. The increase of the initial temperature by a factor of two requires, however, a shock strength $P_s/P_0 \simeq 8$. This shock strength can be provided only by explosions of regions of size $L > 0.5L_d$ (see Figure 6). That is, this effect may slightly decrease the one-dimensional estimate of L_d , but is not likely to change it drastically.

Another effect of a failed initiation on the surrounding material might be the baroclinic generation of additional vorticity [1,42]. Such a secondary source of turbulence reduces the amount of turbulence that must be generated by the primary sources. The turbulent velocity induced by this mechanism may be of order of the postshock velocity. This source of secondary vorticity may be very important in facilitating DDT, but only when the conditions are already close to critical. The amount of secondary vorticity will rapidly decrease with decreasing L . We conclude that our estimate of L_d may decrease by a factor of about two, but will not change drastically if the baroclinic mechanism is taken into account.

The major uncertainty in the estimation of the required turbulent velocity comes from our lack of exact knowledge of flame behavior on scales $\sim x_l$ in the turbulent velocity field. The standard definition of the Gibson scale as the scale at which the turbulent velocity is equal to the laminar flame speed, $U_{\lambda_G} = S_l$, and the assumption that microscopic mixing begins when $\lambda_G = x_l$, gives $K = 1$ in equation (14). As mentioned above, recent work by Poinot et al. [38] and Roberts and Driscoll [39] suggest $K > 1$. There is also some evidence from numerical simulations of turbulent flames that this coefficient might be $K \simeq 3 - 5$, which would increase the critical turbulent velocity accordingly [33]. This must be studied in future numerical simulations and experiments.

The same kind of mixing and flame quenching must also take place in the flame brush of a turbulent deflagration in a tube in order to have DDT in a confined situation. Although shock preconditioning definitely plays an important role in confined situations, there should be a qualitative similarity between triggering detonation by the explosion in the middle of the brush and DDT in unconfined conditions. Carefully planned experiments on DDT in tubes with quantitative characterization of the the turbulent velocity field prior to the explosion in the brush might be used to shed light on the exact value of coefficient K .

4. Conclusions

There are two key elements to the theory presented above for unconfined DDT:

1. *The size of the region L_d that can trigger DDT in a mixture of hot burning product and fuel.* We estimate that $L_d \sim 10^3 x_d$, where x_d is the thickness of the one-dimensional reaction zone of the Chapman-Jouguet detonation, or $L_d \simeq 36 l_c$, where l_c is the detonation cell size, or $L_d \simeq 10^4 x_l$, where x_l is the laminar flame thickness. This implies that large-scale mixing is required to precondition the region.
2. *The intensity of turbulent motions required for the region of size L_d to undergo DDT.* This is estimated from the requirements that the Gibson scale inside this region be comparable to or less than the thickness of the laminar flame (equation 14). This requires the speed of the turbulent flame brush to be $\sim 10^2$ times faster than the laminar flame.

The criterion of DDT in unconfined flames given here can be formulated in terms of the following three parameters of a reactive gas: the one-dimensional thickness of a CJ detonation, x_d , the velocity S_l , and the thickness x_l of the laminar flame. The critical size of the mixed region L_d can be directly related to x_d (Section 2.3), and the latter two parameters determine the critical intensity of turbulence in the mixed region required for triggering DDT (Section 3.1).

The high turbulent velocity required for unconfined DDT is extremely difficult to achieve by turbulence generated by the flame itself or by the Rayleigh-Taylor instability, which explains why DDT in unconfined flames is so hard to observe. The critical size of the region L_d derived in this paper is in agreement with the results of hot jet initiation experiments. The theory may also be extended to confined DDT in the cases when the explosion leading to detonation takes place in the middle of a turbulent flame brush.

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Table 1

Table – Simulated Cases

Case	T_0	γ	q	Q	T_1	T_s	T_d	x_d	L_s/x_d	L_d/x_d
H1	1	1.333	24	28.3	7.0	5.8	10.3	51.2	$\sim 2 \times 10^2$	9.5×10^2
H2	2	1.333	24	28.3	8.0	7.1	11.4	32.3	-	3.3×10^2
H3	3	1.333	24	28.3	9.0	8.3	12.5	23.5	-	$\sim 2 \times 10^2$

T_0	Initial fuel temperature.
γ	Adiabatic index.
q	Total chemical energy release.
Q	Activation energy.
T_1	Temperature of products of isobaric burning.
T_s	Postshock temperature in a Chapman-Jouguet detonation.
T_d	Temperature of Chapman-Jouguet detonation products.
x_d	Half reaction zone length of Chapman-Jouguet detonation.
L_s	Critical length for shock–burning synchronization.
L_d	Critical length for detonation survival in cold fuel.

References

1. Brinkley, S.R., Jr. and Lewis, B., *Seventh Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, pp. 807–811, 1959.
2. Karlovitz, B., *Selected Combustion Problems*, p. 176, London, Butterworths, 1954.
3. Urtiew, P. and Oppenheim, A.K., *Proc. Roy. Soc. Lond. A*, 295:13–28 (1966).
4. Laderman, A.J., Urtiew, P.A. and Oppenheim, A.K., *Ninth Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, p. 265, 1963.
5. Oppenheim, A.K., Laderman, A.J. and Urtiew, P.A., *Combust. Flame*, 6:193–197 (1962).
6. Lee, J.H.S. and Moen, I.O., *Prog. Energy Combust. Sci.*, 6:359–389 (1980).
7. Shepherd, J.E. and Lee, J.H.S., *Major Research Topics in Combustion*, pp. 439–490, eds. M.Y. Hussaini, A. Kumar, and R.G. Voigt, Springer, New York, 1992.
8. Lewis, B. and von Elbe, G., *Combustion, Flames, and Explosions of Gases*, Academic, 1987. 3rd edition, pp. 566–573.
9. Kuo, K.K., *Principles of Combustion*, Wiley, New York, 1986.
10. Zel’dovich, Ya.B., Librovich, V.B., Makhviladze, G.M. and Sivashinsky, G.I., in *2nd International Colloquium on Explosion and Reacting Systems Gasdynamics*, 1969, Aug. 24–29. Novosibirsk, p.10.
11. Zel’dovich, Ya.B., Librovich, V.B., Makhviladze, G.M. and Sivashinsky, G.I., *Astronaut. Acta* 15:313–321 (1970).
12. Lee, J.H.S., Knystautas, R. and Yoshikawa, N., *Acta Astronaut.* 5:971–982 (1978).
13. Yoshikawa, N., *Coherent Shock Wave Amplification in Photochemical Initiation of Gaseous Detonation*, Ph.D. Thesis, Department of Mechanical Engineering, McGill University, 1980.
14. Zel’dovich, Ya.B., Gelfand, B.E., Tsyganov, S.A., Frolov, S.M. and Polenov, A.N., *Progr. Astronaut. Aeronaut.* 114:99–123 (1988).
15. He, L. and Clavin, P., *Twenty-Fourth Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, pp. 1861–1867, 1992.
16. Weber, H.-J., Mack, A. and Roth, P., *Combust. Flame* 97:281–295 (1994).
17. Wagner, H.Gg., in *Proc. Int. Specialist Conf. Fuel-Air Explosions*, U. Waterloo Press, 77–99 (1981).

18. Knystautas, R., Lee, J.H.S., Moen, I.O. and Wagner, H.Gg., *Proceedings of the 17th International Symposium on Combustion*, The Combustion Institute, Pittsburgh, pp. 1235–1245, 1978.
19. Boni, A.A, Chapman, M., Cook, J.L. and Schneyer, J.P., in *Turbulent Combustion*, ed. L. Kennedy, pp. 379–405, (1978).
20. Moen, I.O., Lee, J.H.S., Hjertager, B.H., Fuhre, K. and Eckhoff, R.K., *Combust. Flame* 47:31–52, (1982).
21. Dorofeev., S.B., Bezmelnitsin, A.V., Sidorov, V.P., Yankin, J.G., and Matsukov, I.D., *Fourteenth International Colloquium on Dynamics of Explosions and Reactive Systems*, University of Coimbra, Coimbra, 1993, Vol. 2, pp. D2.4.1–D2.4.10.
22. Carnasciali, F., Lee, J.H.S., and Knystautas, R., *Combust. Flame* 84: 170–180 (1991).
23. Moen, I.O., Bjerketvedt, D., and Jenssen, A., *Combust. Flame* 61: 285–291 (1985).
24. Medvedev, S.P., Polenov, A.N., Khomik, S.V., and Gelfand, B.F., *Twenty-Fifth Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, pp. 73–78, 1994.
25. Khokhlov, A.M., *Astronomy and Astrophys.* 245:114 and 245:L25 (1991).
26. Höflich, P.A., Khokhlov, A.M. and Wheeler, J.C. *Astrophys.J.* 444:831–847 (1994).
27. Zeldovich, Ya.B., and Kompaneets, S.A., *Theory of Detonations*, New York, Academic Press, 1960.
28. Khokhlov, A.M., *Astron. Astrophys.* 246: 383–396 (1991).
29. Strehlow, R., Maurer, R.E. and Rajan, S., *AIAA* 7:323–328 (1969).
30. V. Gamezo (private communication).
31. Colella, P., and Woodward, P.R., *J. Comp. Phys.* 54:174–201 (1984).
32. Colella, P., and Glaz, H.M., *J. Comp. Phys.* 59:264–289 (1985).
33. Khokhlov, A.M., *Astrophys.J.* 449:695–713 (1995).
34. Khokhlov, A.M., Oran, E.S. and Wheeler, J.C., *Combust. Flame* (1996) 105:28–34.
35. Frank-Kamenetskii, D.A., *Diffusion and Heat Transfer in Chemical Kinetics*, Nauka, Moscow (1967).
36. Peters, N., in *Numerical Approaches to Combustion Modeling*, eds. E.S. Oran and J.P. Boris, AIAA, Washington, DC 1991, pp. 155–182.
37. Williams, F.A., in *Mathematics of Combustion*, ed. J.D. Buckmaster, Vol. 2, of *Frontiers in Applied Mathematics*, SIAM, Philadelphia, pp. 97–131 (1985).

- 38. Poinso, T., Veynante, D., and Candel, S., *J. Fluid Mech.* 228: 561–606 (1991).
- 39. Roberts, W.L., and Driscoll, J.F., *Combust. Flame* 87: 245–256 (1991).
- 40. Sung, C.J. (private communication).
- 41. Zel’dovich, Ya.B., *Journ. Applied Mech. Tech. Phys.* 7:68 (1966).
- 42. Picone, J.M., Oran, E.S., Boris, J.P. and Young, T.R. Jr., in *Dynamics of Shock Waves, Explosions, and Detonations*, eds. J.R. Bowen, N. Manson, A.K. Oppenheim, and R.I. Soloukhin, 94, *Prog. Astronaut. Aeronaut.*, 1985, pp. 429–488.

Figure captions

Fig. 1 – (a) Regimes of burning in the $P - V$ plane, ($V = 1/\rho$). Solid curve: detonation adiabat. Dashed curves: shock adiabats. O , initial state of cold fuel; I , state of products of constant volume explosion; CJ , Chapman-Jouguet state; S , unburned post-shock state for CJ detonation; S' , post-shock state for intermediate regime; O' , preshock state for intermediate regime; SP , state of products of spontaneous burning. (b) Schematic of pressure profile of a CJ detonation, spontaneous wave, and intermediate regime. For the spontaneous wave, the pressure changes smoothly from O to CJ , in contrast to the discontinuity $O - S$ in the detonation. In the intermediate regime, pressure increases smoothly from O to O' , and then passes through the shock $O' - S'$.

Fig. 2 – Pressure, velocity, temperature, and reactant concentration as a function of distance at different times (marked by numbers in increasing order) for case H1 (Table 1) with $L/x_d = 30$. Vertical arrow indicates where $D_s p = D_{CJ}$. Values of x_d are given in Table 1.

Fig. 3 – Same as Fig. 1, but with $L/x_d = 300$.

Fig. 4 – Same as Fig. 1, but with $L/x_d = 500$.

Fig. 5 – Same as Fig. 1, but with $L/x_d = 960$.

Fig. 6 – Maximum shock pressure P_s generated during a nonuniform explosion as a function of the length L of a mixed region.